

```
ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 16 17

chain bonds :

3-14

ring bonds :

1-2 1-7 1-8 2-3 2-11 3-4 4-5 5-6 5-16 6-7 6-17 7-12 8-9 8-13

9-10 10-11 12-13

exact/norm bonds :

1-7 2-3 3-4 3-14 4-5 5-6 5-16 6-7 6-17 7-12 8-13 12-13

normalized bonds :

1-2 1-8 2-11 8-9 9-10 10-11
```

G1:0,S,N

Match level:
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom
10:Atom 11:Atom 12:Atom 13:Atom 14:CLASS 16:Atom 17:Atom

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ring nodes:
    1 2 3 4 5 6 7 8 9 10 11 12 13

chain bonds:
    3-14

ring bonds:
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    10-11 12-13

exact/norm bonds:
    1-7 2-3 3-4 3-14 4-5 5-6 6-7 7-12 8-13 12-13

normalized bonds:
    1-2 1-8 2-11 8-9 9-10 10-11
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G1:0,S,N

chain nodes :

Match level:
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:CLASS

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=> d his
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(FILE 'HOME' ENTERED AT 13:10:26 ON 24 MAY 2002)

FILE 'REGISTRY' ENTERED AT 13:11:08 ON 24 MAY 2002

L1 STRUCTURE UPLOADED

L2 QUE L1

L3 15 S L2

L4 SCREEN 1841

L5 STRUCTURE UPLOADED

L6 QUE L5 AND L4

L7 15 S L6

FILE 'STNGUIDE' ENTERED AT 13:12:42 ON 24 MAY 2002

FILE 'REGISTRY' ENTERED AT 13:13:35 ON 24 MAY 2002

L8 SCREEN 1841

L9 STRUCTURE UPLOADED

L10 QUE L9 AND L8

L11 0 S L10

L12 252 S L6 SSS FUL

L13 1 S L10 SUB=L12 FUL

FILE 'CAPLUS' ENTERED AT 13:14:23 ON 24 MAY 2002

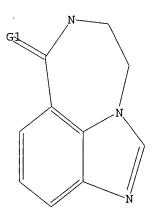
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L16 5 S L14 OR L15

=> d 16

L6 HAS NO ANSWERS

L4 SCR 1841 L5 STR



G1 O, S, N

Structure attributes must be viewed using STN Express query preparation. L6 QUE ABB=ON PLU=ON L5 AND L4

=> d 110

L10 HAS NO ANSWERS

L8 SCR 1841

Page 1

G1 O, S, N

L9 STR

Structure attributes must be viewed using STN Express query preparation. L10 $$\tt QUE $\tt ABB=ON $\tt PLU=ON $\tt L9 $\tt AND $\tt L8 \tt

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ANSWER 1 OF 5 CAPLUS COPYRIGHT 2002 ACS
     2001:225212
                   CAPLUS
     134:266331
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ΤI
     Preparation of 2-phenyl-5,6-dihydro-imidazo[4,5,1-jk][1,4]benzodiazepin-
     7(4H)-ones as poly(ADP ribose) polymerase inhibitors.
     Lubisch, Wilfried; Kock, Michael; Hoeger, Thomas; Grandel, Roland;
IN
     Mueller, Reinhold; Schult, Sabine
PA
     BASF A.-G., Germany
SO
     Ger. Offen., 12 pp.
     CODEN: GWXXBX
DT
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     German
LА
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                        KIND DATE
                                                APPLICATION NO.
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     MARPAT 134:266331
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AB Title compds. [I; A = (substituted) C1-3 alkylene; X1 = S, O, NE; X2 = N, (substituted) C; X3 = N, CR2; R2 = H, alkyl, alkylphenyl, Ph; R1 = H, halo, OH, NO2, CF3, cyano, alkyl, alkoxy, etc.; B = (unsatd.) (O-, N-, S-interrupted) (substituted) mono-, bi-, tricyclyl] were prepd. as poly(ADP ribose) polymerase inhibitors (no data). Thus, Me 2-chloro-3-nitrobenzoate was heated with K2CO3 and H2NCH2CH2NH2 in DMF for 3 at 120.degree. to give 9-nitro-1,2,3,4-tetrahydro-5H-1,4-benzodiazepin-5-one, which was hydrogenated using Pd/C in EtOH to give 9-amino-1,2,3,4-tetrahydro-5H-1,4-benzodiazepin-5-one. The latter in MeOH contg. HOAc was treated dropwise with 4-(4-methylpiperazin-1-yl)benzaldehyde in MeOH followed by 1 h stirring at room temp.; Cu(OAc)2, Na2S, and HCl in H2O were added followed by 30 min reflux to give 2-[4-(4-methylpiperazin-1-yl)phenyl]-5,6-dihydro-imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one.

IT 331730-18-8P 331730-20-2P 331730-21-3P 331730-22-4P 331730-23-5P 331730-24-6P 331730-26-8P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of phenyldihydroimidazobenzodiazepinones as PARP inhibitors)

RN 331730-18-8 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-(4-methyl-1-piperazinyl)phenyl]- (9CI) (CA INDEX NAME)

RN 331730-20-2 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-[2-(diethylamino)ethoxy]phenyl]-5,6-dihydro-(9CI) (CA INDEX NAME)

RN 331730-21-3 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-[2-(1-piperidinyl)ethoxy]phenyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

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RN 331730-22-4 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-[2-

(diethylamino)ethyl]methylamino]phenyl]-5,6-dihydro- (9CI) (CA INDEX NAME)

RN 331730-23-5 CAPLUS

CN 1-Piperazinecarboxylic acid, 4-[4-(4,5,6,7-tetrahydro-7-oxoimidazo[4,5,1-jk][1,4]benzodiazepin-2-yl)phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 331730-24-6 CAPLUS

CN 1H-1,4-Diazepine-1-carboxylic acid, hexahydro-4-[4-(4,5,6,7-tetrahydro-7-oxoimidazo[4,5,1-jk][1,4]benzodiazepin-2-yl)phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 331730-26-8 CAPLUS

CN 1H-1,4-Diazepine-1-carboxylic acid, hexahydro-4-[4-(4,5,6,7-tetrahydro-7-oxoimidazo[4,5,1-jk][1,4]benzodiazepin-2-yl)phenyl]-, 1,1-dimethylethyl ester, trihydrochloride (9CI) (CA INDEX NAME)

IT 331730-19-9

RL: RCT (Reactant); RACT (Reactant or reagent) (prepn. of phenyldihydroimidazobenzodiazepinones as PARP inhibitors) 331730-19-9 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-(4-

RN

nitrophenyl) - (9CI) (CA INDEX NAME)

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ANSWER 2 OF 5 CAPLUS COPYRIGHT 2002 ACS
      2001:167995 CAPLUS
      134:207833
      Preparation of tricyclic inhibitors of poly(ADP-ribose) polymerases
ΤI
IN
      Webber, Stephen Evan; Skalitzky, Donald James; Tikhe, Jayashree Girish;
      Kumpf, Robert Arnold; Marakovits, Joseph Timothy; Eastman, Walter Brian
PΑ
      Agouron Pharmaceuticals, Inc., USA; Cancer Research Campaign Technology
      Limited
SO
      PCT Int. Appl., 236 pp.
      CODEN: PIXXD2
DT
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FAN.CNT 1
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PRAI US 1999-152142P
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      MARPAT 134:207833
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$$R^2$$
 R^5
 R^6
 R^7
 R^8
 R^8
 R^4
 R^4
 R^5

The title compds. [I; X = O, S; Y = N, CR3 (wherein R3 = halo, CN, alkyl, AΒ etc.); R1 = H, halo, CN, etc.; R2 = H, alkyl; R4 = H, halo, alkyl; R5-R8 = H, alkyl, alkenyl, aryl, etc.] which are poly(ADP-ribosyl)transferase inhibitors, and are useful in treating cancers and in ameliorating the effects of stroke, head trauma, and neurodegenerative disease, were prepd. E.g., a multi-step synthesis of 1-phenyl-8,9-dihydro-7H-2,7,9a-triazabenzo[cd]azulen-6-one [I; Y = N; X = O; R1 = Ph; R2, R4-R8 = H] was given. Biol. data for compds. I were presented. IT 328542-04-7P 328542-20-7P 328542-32-1P 328542-58-1P 328542-59-2P 328542-61-6P 328543-05-1P 328543-07-3P 328543-09-5P 328543-29-9P 328543-31-3P 328543-50-6P 328543-84-6P 328544-00-9P 328544-08-7P 328544-29-2P 328544-34-9P 328544-38-3P 328544-40-7P 328544-42-9P 328544-48-5P

328544-55-4P 328544-57-6P 328544-61-2P 328544-71-4P 328544-77-0P 328544-83-8P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(prepn. of tricyclic inhibitors of poly(ADP-ribose) polymerases) RN 328542-04-7 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-phenyl- (9CI) (CA INDEX NAME)

RN 328542-20-7 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-(1-naphthalenyl)- (9CI) (CA INDEX NAME)

RN 328542-32-1 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-(2-chloro-4-pyridinyl)-5,6-dihydro-(9CI) (CA INDEX NAME)

RN 328542-58-1 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[(phenylmethyl)thio]- (9CI) (CA INDEX NAME)

RN 328542-59-2 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[3-(1,3-dioxan-2-yl)phenyl]-5,6-dihydro-(9CI) (CA INDEX NAME)

RN 328542-61-6 CAPLUS

CN Benzaldehyde, 3-(4,5,6,7-tetrahydro-7-oxoimidazo[4,5,1-jk][1,4]benzodiazepin-2-yl)- (9CI) (CA INDEX NAME)

RN 328543-05-1 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-(diethoxymethyl)phenyl]-5,6-dihydro-(9CI) (CA INDEX NAME)

RN 328543-07-3 CAPLUS CN Benzaldehyde, 4-(4,5,6,7-tetrahydro-7-oxoimidazo[4,5,1-jk][1,4]benzodiazepin-2-yl)- (9CI) (CA INDEX NAME)

RN 328543-09-5 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4[(dimethylamino)methyl]phenyl]-5,6-dihydro- (9CI) (CA INDEX NAME)

RN 328543-29-9 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[3-(1,3-dioxolan-2-yl)phenyl]-9-fluoro-5,6-dihydro- (9CI) (CA INDEX NAME)

RN 328543-31-3 CAPLUS CN Benzaldehyde, 3-(9-fluoro-4,5,6,7-tetrahydro-7-oxoimidazo[4,5,1-jk][1,4]benzodiazepin-2-yl)- (9CI) (CA INDEX NAME)

RN 328543-50-6 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-(diethoxymethyl)phenyl]-9-fluoro-5,6-dihydro-(9CI) (CA INDEX NAME)

RN 328543-84-6 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 9-fluoro-5,6-dihydro-2-[4-(hydroxymethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 328544-00-9 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-(4-thiomorpholinylmethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 328544-08-7 CAPLUS

CN Benzonitrile, 4-[[5-(4,5,6,7-tetrahydro-7-oxoimidazo[4,5,1-jk][1,4]benzodiazepin-2-yl)-2-pyridinyl]oxy]- (9CI) (CA INDEX NAME)

RN 328544-29-2 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-(2-hydroxyethoxy)phenyl]- (9CI) (CA INDEX NAME)

RN 328544-34-9 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-[2-(1-pyrrolidinyl)ethoxy]phenyl]- (9CI) (CA INDEX NAME)

RN 328544-38-3 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-[2-(tetrahydro-2H-pyran-2-yl)ethyl]phenyl]- (9CI) (CA INDEX NAME)

RN 328544-40-7 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-(2-pyridinyl)phenyl]- (9CI) (CA INDEX NAME)

RN 328544-42-9 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-(2-hydroxyethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 328544-48-5 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-(2-piperidinyl)phenyl]- (9CI) (CA INDEX NAME)

RN 328544-55-4 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-(3-pyridinyl)phenyl]- (9CI) (CA INDEX NAME)

RN 328544-57-6 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-(4-pyridinyl)phenyl]- (9CI) (CA INDEX NAME)

RN 328544-61-2 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-(4-piperidinyl)phenyl]- (9CI) (CA INDEX NAME)

RN 328544-71-4 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-(3-piperidinyl)phenyl]- (9CI) (CA INDEX NAME)

RN 328544-77-0 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[(phenylmethyl)amino]- (9CI) (CA INDEX NAME)

RN 328544-83-8 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-(2-pyrrolidinyl)phenyl]- (9CI) (CA INDEX NAME)

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     study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
     BIOL (Biological study); PREP (Preparation); USES (Uses)
        (prepn. of tricyclic inhibitors of poly(ADP-ribose) polymerases)
RN
     328542-06-9 CAPLUS
CN
     Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-(4-fluorophenyl)-5,6-
     dihydro- (9CI) (CA INDEX NAME)
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RN 328542-08-1 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-(4-pyridinyl)-
(9CI) (CA INDEX NAME)
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RN 328542-10-5 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-(3,4-difluorophenyl)-5,6-dihydro- (9CI) (CA INDEX NAME)

RN 328542-12-7 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-(2-chlorophenyl)-5,6-dihydro- (9CI) (CA INDEX NAME)

RN 328542-14-9 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-(3-phenoxyphenyl)- (9CI) (CA INDEX NAME)

RN 328542-16-1 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-(3-pyridinyl)-(9CI) (CA INDEX NAME)

RN 328542-18-3 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-(2-thienyl)-(9CI) (CA INDEX NAME)

RN 328542-22-9 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

10/041,556

RN 328542-24-1 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

RN 328542-26-3 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-(2-pyridinyl)-(9CI) (CA INDEX NAME)

RN 328542-28-5 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-(5-isoxazolyl)- (9CI) (CA INDEX NAME)

RN 328542-30-9 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-(4-chlorophenyl)-5,6-dihydro- (9CI) (CA INDEX NAME)

RN 328542-34-3 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[3-(3-pyridinyloxy)phenyl]- (9CI) (CA INDEX NAME)

RN 328542-36-5 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[3-(4-pyridinyloxy)phenyl]- (9CI) (CA INDEX NAME)

RN 328542-38-7 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 9-fluoro-2-(4-fluorophenyl)-5,6-dihydro-(9CI) (CA INDEX NAME)

RN 328542-40-1 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-(2-phenylethyl)- (9CI) (CA INDEX NAME)

RN 328542-42-3 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-(2-furanyl)-5,6-dihydro-(9CI) (CA INDEX NAME)

RN 328542-43-4 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 328542-48-9 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-cyclohexyl-5,6-dihydro-(9CI) (CA INDEX NAME)

RN 328542-50-3 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepine-7(4H)-thione, 5,6-dihydro-2-phenyl-(9CI) (CA INDEX NAME)

RN 328542-54-7 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-6-methyl-2-(1-naphthalenyl)- (9CI) (CA INDEX NAME)

RN 328542-63-8 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[3-[(dimethylamino)methyl]phenyl]-5,6-dihydro-(9CI) (CA INDEX NAME)

RN 328542-99-0 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepine-2,7(1H,4H)-dione, 5,6-dihydro-4-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)

RN 328543-01-7 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-(4-chlorophenyl)-5,6-dihydro-4-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)

RN 328543-03-9 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[3-(1,3-dioxolan-2-yl)phenyl]-5,6-dihydro- (9CI) (CA INDEX NAME)

RN 328543-11-9 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[3-[(methylamino)methyl]phenyl]- (9CI) (CA INDEX NAME)

RN 328543-13-1 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[3-(1-pyrrolidinylmethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 328543-15-3 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[3-[3-(trifluoromethyl)phenoxy]phenyl]- (9CI) (CA INDEX NAME)

RN 328543-17-5 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[3-(4-chlorophenoxy)phenyl]-5,6-dihydro- (9CI) (CA INDEX NAME)

RN 328543-19-7 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[3-(3,4-dichlorophenoxy)phenyl]-5,6-dihydro- (9CI) (CA INDEX NAME)

RN 328543-21-1 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[3-(4-methoxyphenoxy)phenyl]- (9CI) (CA INDEX NAME)

RN 328543-23-3 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[3-(3,5-dichlorophenoxy)phenyl]-5,6-dihydro-(9CI) (CA INDEX NAME)

RN 328543-25-5 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-(3-benzoylphenyl)-5,6-dihydro- (9CI) (CA INDEX NAME)

RN 328543-27-7 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[3-(phenylmethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 328543-33-5 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[3-[(dimethylamino)methyl]phenyl]-9-fluoro-5,6-dihydro-(9CI) (CA INDEX

NAME)

RN 328543-35-7 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[2-(dimethylamino)-4-pyridinyl]-5,6-dihydro- (9CI) (CA INDEX NAME)

RN 328543-37-9 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 9-fluoro-5,6-dihydro-2-[3-[(methylamino)methyl]phenyl]- (9CI) (CA INDEX NAME)

RN 328543-39-1 CAPLUS

CN Benzonitrile, 3-(4,5,6,7-tetrahydro-7-oxoimidazo[4,5,1-jk][1,4]benzodiazepin-2-yl)- (9CI) (CA INDEX NAME)

RN 328543-43-7 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-[(methylamino)methyl]phenyl]- (9CI) (CA INDEX NAME)

RN 328543-45-9 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-(4-morpholinylmethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 328543-47-1 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-[[(2-methoxyethyl)amino]methyl]phenyl]- (9CI) (CA INDEX NAME)

RN 328543-49-3 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-(4-phenoxyphenyl)- (9CI) (CA INDEX NAME)

RN 328543-52-8 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-(1H-imidazol-2-yl)- (9CI) (CA INDEX NAME)

RN 328543-78-8 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-(2-thiazolyl)-(9CI) (CA INDEX NAME)

RN 328543-80-2 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-(1H-pyrrol-2-yl)- (9CI) (CA INDEX NAME)

RN 328543-82-4 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[5-(4-chlorophenyl)-2-furanyl]-5,6-dihydro- (9CI) (CA INDEX NAME)

RN 328543-86-8 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 9-fluoro-5,6-dihydro-2-[4-[(methylamino)methyl]phenyl]- (9CI) (CA INDEX NAME)

RN 328543-89-1 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4[(dimethylamino)methyl]phenyl]-9-fluoro-5,6-dihydro- (9CI) (CA INDEX NAME)

RN 328543-91-5 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-[[(2-ethoxyethyl)amino]methyl]phenyl]-5,6-dihydro- (9CI) (CA INDEX NAME)

RN 328543-92-6 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4[(cyclopropylamino)methyl]phenyl]-5,6-dihydro- (9CI) (CA INDEX NAME)

RN 328543-94-8 CAPLUS
CN Acetonitrile, [[[4-(4,5,6,7-tetrahydro-7-oxoimidazo[4,5,1-jk][1,4]benzodiazepin-2-yl)phenyl]methyl]amino]- (9CI) (CA INDEX NAME)

RN 328543-96-0 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-[[(2,2,2-trifluoroethyl)amino]methyl]phenyl]- (9CI) (CA INDEX NAME)

RN 328543-98-2 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-[(2-propynylamino)methyl]phenyl]- (9CI) (CA INDEX NAME)

$$HC \equiv C - CH_2 - NH - CH_2$$
 N
 N
 N
 N
 N

RN 328544-02-1 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[2-(4-methylphenyl)-4-thiazolyl]- (9CI) (CA INDEX NAME)

RN 328544-04-3 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[3-(4-methylphenyl)-2,1-benzisoxazol-5-yl]- (9CI) (CA INDEX NAME)

RN 328544-06-5 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[6-[(4-chlorophenyl)thio]-3-pyridinyl]-5,6-dihydro- (9CI) (CA INDEX NAME)

RN 328544-10-1 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepine-2-carboxamide, 4,5,6,7-tetrahydro-7-oxo-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 328544-12-3 CAPLUS

CN Propanenitrile, 3-[[[4-(4,5,6,7-tetrahydro-7-oxoimidazo[4,5,1-jk][1,4]benzodiazepin-2-yl)phenyl]methyl]amino]- (9CI) (CA INDEX NAME)

RN 328544-16-7 CAPLUS
CN Morpholine, 4-[(4,5,6,7-tetrahydro-7-oxoimidazo[4,5,1-jk][1,4]benzodiazepin-2-yl)carbonyl]- (9CI) (CA INDEX NAME)

RN 328544-18-9 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[1,6-dihydro-6-oxo-1-(phenylmethyl)-3-pyridinyl]-5,6-dihydro-(9CI) (CA INDEX NAME)

RN 328544-20-3 CAPLUS
CN Piperazine, 1-methyl-4-[(4,5,6,7-tetrahydro-7-oxoimidazo[4,5,1-jk][1,4]benzodiazepin-2-yl)carbonyl]- (9CI) (CA INDEX NAME)

RN 328544-22-5 CAPLUS
CN Benzamide, 4-[[5-(4,5,6,7-tetrahydro-7-oxoimidazo[4,5,1-jk][1,4]benzodiazepin-2-yl)-2-pyridinyl]oxy]- (9CI) (CA INDEX NAME)

RN 328544-23-6 CAPLUS CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-tricyclo[3.3.1.13,7]dec-1-yl- (9CI) (CA INDEX NAME)

RN 328544-25-8 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-(6-chloro-3-pyridinyl)-5,6-dihydro- (9CI) (CA INDEX NAME)

RN 328544-27-0 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-(1H-imidazol-1-yl)phenyl]- (9CI) (CA INDEX NAME)

RN 328544-31-6 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-[3-(dimethylamino)propoxy]phenyl]-5,6-dihydro-(9CI) (CA INDEX NAME)

RN 328544-33-8 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-[(1-oxido-4-thiomorpholinyl)methyl]phenyl]- (9CI) (CA INDEX NAME)

RN 328544-36-1 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-[2-(dimethylamino)ethoxy]phenyl]-5,6-dihydro-(9CI) (CA INDEX NAME)

RN 328544-44-1 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-[2-(1-pyrrolidinyl)ethyl]phenyl]- (9CI) (CA INDEX NAME)

RN 328544-46-3 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-[2-(dimethylamino)ethyl]phenyl]-5,6-dihydro-(9CI) (CA INDEX NAME)

RN 328544-49-6 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4[(dimethyloxidoamino)methyl]phenyl]-5,6-dihydro- (9CI) (CA INDEX NAME)

RN 328544-51-0 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-(1-methyl-2-piperidinyl)phenyl]- (9CI) (CA INDEX NAME)

RN 328544-53-2 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-(2-methyl-2H-tetrazol-5-yl)phenyl]- (9CI) (CA INDEX NAME)

RN 328544-59-8 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-(1H-tetrazol-5-yl)phenyl]- (9CI) (CA INDEX NAME)

RN 328544-69-0 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-(1-methyl-4-piperidinyl)phenyl]- (9CI) (CA INDEX NAME)

RN 328544-73-6 CAPLUS

CN 1-Piperidinecarboxylic acid, 3-[4-(4,5,6,7-tetrahydro-7-oxoimidazo[4,5,1-jk][1,4]benzodiazepin-2-yl)phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 328544-75-8 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-(1-methyl-3-piperidinyl)phenyl]- (9CI) (CA INDEX NAME)

RN 328544-81-6 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-(1H-imidazol-4-yl)phenyl]- (9CI) (CA INDEX NAME)

RN328544-85-0 CAPLUS

Imidazo[4,5,1-jk][1,4] benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-(1-methyl-meCN2-pyrrolidinyl)phenyl]- (9CI) (CA INDEX NAME)

RN

 $328544-87-2 \quad \text{CAPLUS} \\ \text{Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, } 2-[4-[1-(cyclopropylmethyl)-2-piperidinyl]phenyl]-5,6-dihydro- (9CI) (CA INDEX NAME) \\$ CN

RN 328544-89-4 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-[1-(1-methylethyl)-2-piperidinyl]phenyl]- (9CI) (CA INDEX NAME)

RN 328544-91-8 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-(1H-imidazol-2-yl)phenyl]- (9CI) (CA INDEX NAME)

10/041,556

RN 328545-24-0 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-[(2,5-dihydro-1H-pyrrol-1-yl)methyl]phenyl]-5,6-dihydro-(9CI) (CA INDEX NAME)

RN 328545-25-1 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 9-fluoro-5,6-dihydro-2-[4-[(3-hydroxy-1-pyrrolidinyl)methyl]phenyl]- (9CI) (CA INDEX NAME)

RN 328545-28-4 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-[[(2R)-2-(hydroxymethyl)-1-pyrrolidinyl]methyl]phenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 328545-30-8 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-[(3-hydroxy-1-pyrrolidinyl)methyl]phenyl]- (9CI) (CA INDEX NAME)

RN 328545-31-9 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-[[3-(hydroxymethyl)-1-piperidinyl]methyl]phenyl]- (9CI) (CA INDEX NAME)

RN 328545-33-1 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-[[(2,3-dihydroxypropyl)methylamino]methyl]phenyl]-5,6-dihydro- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{OH} & \text{Me} \\ & & \\ \text{HO-CH}_2 - \text{CH-CH}_2 - \text{N-CH}_2 \\ \hline & & \\ &$$

RN 328545-34-2 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-[(2,5-dihydro-1H-pyrrol-1-yl)methyl]phenyl]-9-fluoro-5,6-dihydro-(9CI) (CA INDEX NAME)

RN 328545-37-5 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-[[4-(2-propenyl)-1-piperazinyl]methyl]phenyl]-, trifluoroacetate (5:4) (9CI) (CA INDEX NAME)

CM 1

CRN 328545-36-4 CMF C24 H27 N5 O

CRN 76-05-1 CMF C2 H F3 O2

RN 328545-40-0 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-[[methyl(2-phenylethyl)amino]methyl]phenyl]-, trifluoroacetate (5:3) (9CI) (CA INDEX NAME)

CM 1

CRN 328545-39-7 CMF C26 H26 N4 O

$$\begin{array}{c} \text{Me} \\ \\ \text{Ph-CH}_2 - \text{CH}_2 - \text{N-CH}_2 \\ \\ \\ \text{N} \\ \\ \text{N} \\ \\ \text{O} \end{array}$$

CRN 76-05-1 CMF C2 H F3 O2

RN 328545-43-3 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-[[butyl(2-hydroxyethyl)amino]methyl]phenyl]-5,6-dihydro-, trifluoroacetate (5:3) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 328545-42-2 CMF C23 H28 N4 O2

CRN 76-05-1 CMF C2 H F3 O2

RN 328545-46-6 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-[[(2S)-2-(hydroxymethyl)-1-pyrrolidinyl]methyl]phenyl]-, mono(trifluoroacetate) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 328545-45-5 CMF C22 H24 N4 O2

Absolute stereochemistry.

CRN 76-05-1 CMF C2 H F3 O2

CN

RN 328545-48-8 CAPLUS

Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, -2-[4-[(3,6-dihydro-1(2H)pyridinyl)methyl]phenyl]-5,6-dihydro-, trifluoroacetate (20:17) (9CI) (CA
INDEX NAME)

CM 1

CRN 328545-47-7 CMF C22 H22 N4 O

CRN 76-05-1 CMF C2 H F3 O2

RN 328545-51-3 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-[[(2-phenylethyl)amino]methyl]phenyl]-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 328545-50-2 CMF C25 H24 N4 O

CRN 76-05-1 CMF C2 H F3 O2

RN 328545-54-6 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-[[[2-(3-methoxyphenyl)ethyl]amino]methyl]phenyl]-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 328545-53-5 CMF C26 H26 N4 O2

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CM 2

CRN 76-05-1

CMF C2 H F3 O2

RN 328545-57-9 CAPLUS CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-[[[2-(4-

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fluorophenyl)ethyl]amino]methyl]phenyl]-5,6-dihydro-, trifluoroacetate
(5:8) (9CI) (CA INDEX NAME)

CM 1

CRN 328545-56-8 CMF C25 H23 F N4 O

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PAGE 2-A

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 328545-60-4 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-[[[2-(4-methoxyphenyl)ethyl]amino]methyl]phenyl]-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 328545-59-1 CMF C26 H26 N4 O2

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PAGE 2-A

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 328545-63-7 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-[[methyl(2-methylpropyl)amino]methyl]phenyl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 328545-62-6 CMF C22 H26 N4 O

CM 2

CRN 76-05-1 CMF C2 H F3 O2

CM 1

CRN 328545-65-9 CMF C21 H22 N4 O

CM 2

CRN 76-05-1 CMF C2 H F3 O2

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RN
    328545-69-3 CAPLUS
    CN
    INDEX NAME)
    CM
        1
    CRN 328545-68-2
    CMF C22 H20 N4 O S
 ΝН
 CH<sub>2</sub>
    CM
        2
        76-05-1
    CRN
        C2 H F3 O2
    CMF
    CO2H
RN
    328545-72-8 CAPLUS
CN
    Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-
    [(dipropylamino)methyl]phenyl]-5,6-dihydro-, bis(trifluoroacetate) (9CI)
    (CA INDEX NAME)
    CM
        1
        328545-71-7
    CRN
    CMF
        C23 H28 N4 O
```

CRN 76-05-1 CMF C2 H F3 O2

RN 328545-75-1 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-[[(1,3-benzodioxol-5-ylmethyl)amino]methyl]phenyl]-5,6-dihydro-, trifluoroacetate (4:9) (9CI) (CA INDEX NAME)

CM 1

CRN 328545-74-0 CMF C25 H22 N4 O3

CRN 76-05-1 CMF C2 H F3 O2

RN 328545-78-4 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-[[(2,3-dihydro-1H-inden-1-yl)amino]methyl]phenyl]-5,6-dihydro-, trifluoroacetate (10:19) (9CI) (CA INDEX NAME)

CM 1

CRN 328545-77-3 CMF C26 H24 N4 O

CRN 76-05-1 CMF C2 H F3 O2

CN

RN 328545-81-9 CAPLUS

.beta.-Alanine, N-(2-furanylmethyl)-N-[[4-(4,5,6,7-tetrahydro-7-oxoimidazo[4,5,1-jk][1,4]benzodiazepin-2-yl)phenyl]methyl]-, ethyl ester, trifluoroacetate (4:7) (9CI) (CA INDEX NAME)

CM 1

CRN 328545-80-8 CMF C27 H28 N4 O4

CRN 76-05-1 CMF C2 H F3 O2

RN 328545-84-2 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-[[[2-(1-methyl-2-pyrrolidinyl)ethyl]amino]methyl]phenyl]-, trifluoroacetate (4:13) (9CI) (CA INDEX NAME)

CM 1

CRN 328545-83-1 CMF C24 H29 N5 O

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. CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 328545-86-4 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-[[[(5-i)]]]

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methyl-2-furanyl)methyl]amino]methyl]phenyl]-, trifluoroacetate (4:5)
(9CI) (CA INDEX NAME)

CM 1

CRN 328545-85-3 CMF C23 H22 N4 O2

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CM 2

CRN 76-05-1 CMF C2 H F3 O2

F-C-CO₂H

RN 328545-89-7 CAPLUS

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CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-[(phenylmethyl)amino]methyl]phenyl]-, trifluoroacetate (2:3) (9CI) (CA INDEX NAME)

CM 1

CRN 328545-88-6 CMF C24 H22 N4 O

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 328545-91-1 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-[[(2,3-dihydro-1H-inden-2-yl)amino]methyl]phenyl]-5,6-dihydro-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 328545-90-0 CMF C26 H24 N4 O

CRN 76-05-1 CMF C2 H F3 O2

RN 328545-94-4 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-[(3,4-dihydro-2(1H)-isoquinolinyl)methyl]phenyl]-5,6-dihydro-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 328545-93-3 CMF C26 H24 N4 O

CRN 76-05-1 CMF C2 H F3 O2

RN 328545-97-7 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-[[methyl(phenylmethyl)amino]methyl]phenyl]-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 328545-96-6 CMF C25 H24 N4 O

CRN 76-05-1 CMF C2 H F3 O2

CN

RN 328545-99-9 CAPLUS

Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-[[(2-phenylpropyl)amino]methyl]phenyl]-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 328545-98-8 CMF C26 H26 N4 O

CRN 76-05-1 CMF C2 H F3 O2

RN 328546-02-7 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-[[(3-phenylpropyl)amino]methyl]phenyl]-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 328546-01-6 CMF C26 H26 N4 O

CRN 76-05-1 CMF C2 H F3 O2

RN 328546-05-0 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-[[methyl[2-(2-pyridinyl)ethyl]amino]methyl]phenyl]-, tris(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 328546-04-9 CMF C25 H25 N5 O

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CM 2

CRN 76-05-1 CMF C2 H F3 O2

F-C-CO₂F

RN 328546-07-2 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-[[ethyl[2-(2-10])]]

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pyridinyl)ethyl]amino]methyl]phenyl]-5,6-dihydro-, tris(trifluoroacetate)
(9CI) (CA INDEX NAME)

CM 1

CRN 328546-06-1 CMF C26 H27 N5 O

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CM 2

CRN 76-05-1 CMF C2 H F3 O2

CN

RN 328546-09-4 CAPLUS

Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-[[[2-(2-pyridinyl)ethyl]amino]methyl]phenyl]-, trifluoroacetate (4:9) (9CI) (CA INDEX NAME)

CM 1

CRN 328546-08-3 CMF C24 H23 N5 O

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CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 328546-13-0 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-[[methyl[2-(4-pyridinyl)ethyl]amino]methyl]phenyl]-, trifluoroacetate (2:7) (9CI) (CA INDEX NAME)

CM 1

CRN 328546-12-9 CMF C25 H25 N5 O

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CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 328546-15-2 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-[[[2-(4-k-1)]]])

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pyridinyl)ethyl]amino]methyl]phenyl]-, trifluoroacetate (4:13) (9CI) (CA INDEX NAME)

CM 1

CRN 328546-14-1 CMF C24 H23 N5 O

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CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 328546-17-4 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-[[[2-(1H-indol-2-yl)ethyl]methylamino]methyl]phenyl]-, trifluoroacetate (2:5) (9CI) (CA INDEX NAME)

CM 1

CRN 328546-16-3 CMF C28 H27 N5 O

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 328546-18-5 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-(azidomethyl)phenyl]-5,6-dihydro-(9CI) (CA INDEX NAME)

10/041,556

RN 328546-20-9 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-(aminomethyl)phenyl]-5,6-dihydro-, trifluoroacetate (4:7) (9CI) (CA INDEX NAME)

CM 1

CRN 328546-19-6 CMF C17 H16 N4 O

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 328546-21-0 CAPLUS CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-(1-

Page 91

pyrrolidinylmethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 328546-22-1 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 9-fluoro-5,6-dihydro-2-[4-(1-pyrrolidinylmethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 328546-23-2 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-[(2-methyl-1-pyrrolidinyl)methyl]phenyl]- (9CI) (CA INDEX NAME)

RN 328546-25-4 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-(1H-imidazol-1-ylmethyl)phenyl]-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 328546-24-3 CMF C20 H17 N5 O

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 328546-26-5 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-[(2,5-dimethyl-1-pyrrolidinyl)methyl]phenyl]-5,6-dihydro- (9CI) (CA INDEX NAME)

RN 328546-27-6 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-[(1,3,3-trimethyl-6-azabicyclo[3.2.1]oct-6-yl)methyl]phenyl]- (9CI) (CA INDEX NAME)

RN 328546-28-7 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-[[(2S,5S)-2,5-bis(methoxymethyl)-1-pyrrolidinyl]methyl]phenyl]-5,6-dihydro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 328546-29-8 CAPLUS
CN D-Proline, 1-[[4-(4,5,6,7-tetrahydro-7-oxoimidazo[4,5,1-jk][1,4]benzodiazepin-2-yl)phenyl]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 328546-31-2 CAPLUS

CN D-Proline, 1-[[4-(4,5,6,7-tetrahydro-7-oxoimidazo[4,5,1-jk][1,4]benzodiazepin-2-yl)phenyl]methyl]-, 1,1-dimethylethyl ester, trifluoroacetate (4:3) (9CI) (CA INDEX NAME)

CM 1

CRN 328546-30-1 CMF C26 H30 N4 O3

Absolute stereochemistry.

CM 2

CRN 76-05-1 CMF C2 H F3 O2

CN

RN 328546-32-3 CAPLUS

Carbamic acid, [1-[[4-(4,5,6,7-tetrahydro-7-oxoimidazo[4,5,1-jk][1,4]benzodiazepin-2-yl)phenyl]methyl]-3-pyrrolidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 328546-33-4 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-(1H-pyrrol-1-ylmethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 328546-34-5 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4[(dimethylamino)methyl]phenyl]-5,6-dihydro-5-methyl-, (5S)- (9CI) (CA
INDEX NAME)

Absolute stereochemistry.

RN 328546-36-7 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-5-methyl-2-[4-[(methylamino)methyl]phenyl]-, (5S)-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 328546-35-6 CMF C19 H20 N4 O

Absolute stereochemistry.

CRN 76-05-1 CMF C2 H F3 O2

RN 328546-38-9 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-[(2,5-dihydro-1H-pyrrol-1-yl)methyl]phenyl]-5,6-dihydro-5-methyl-, (5S)-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1 .

CRN 328546-37-8 CMF C22 H22 N4 O

Absolute stereochemistry.

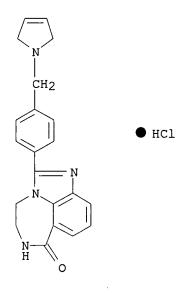
10/041,556

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 328546-39-0 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-[(2,5-dihydro-1H-pyrrol-1-yl)methyl]phenyl]-5,6-dihydro-, monohydrochloride (9CI) (CA INDEX NAME)



RN 328546-40-3 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-[(2,5-dihydro-1H-pyrrol-1-yl)methyl]phenyl]-5,6-dihydro-, (2Z)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 328545-24-0 CMF C21 H20 N4 O

CRN 110-16-7 CMF C4 H4 O4 CDES 2:Z

Double bond geometry as shown.

RN 328546-41-4 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-[(2,5-dihydro-1H-pyrrol-1-yl)methyl]phenyl]-5,6-dihydro-, monomethanesulfonate (9CI) (CA INDEX NAME)

CM 1

CRN 328545-24-0 CMF C21 H20 N4 O 10/041,556

CM 2

CRN 75-75-2 CMF C H4 O3 S

RN 328546-42-5 CAPLUS

CN Benzonitrile, 4-(4,5,6,7-tetrahydro-7-oxoimidazo[4,5,1-jk][1,4]benzodiazepin-2-yl)- (9CI) (CA INDEX NAME)

RN 328546-43-6 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-(1-hydroxy-1)]

3-methylbutyl)phenyl]- (9CI) (CA INDEX NAME)

RN 328546-44-7 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-[1-(2,5-dihydro-1H-pyrrol-1-yl)-3-methylbutyl]phenyl]-5,6-dihydro-(9CI) (CA INDEX NAME)

RN 328546-45-8 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-[3-methyl-1-(1-pyrrolidinyl)butyl]phenyl]- (9CI) (CA INDEX NAME)

RN 328546-46-9 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-[1-(dimethylamino)-3-methylbutyl]phenyl]-5,6-dihydro- (9CI) (CA INDEX NAME)

RN 328546-47-0 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-[(2,5-dihydro-1H-pyrrol-1-yl)methyl]phenyl]-9-fluoro-5,6-dihydro-, monomethanesulfonate (9CI) (CA INDEX NAME)

CM 1

CRN 328545-34-2 CMF C21 H19 F N4 O 10/041,556

CM 2

CRN 75-75-2 CMF C H4 O3 S

RN 328546-48-1 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-5-methyl-2-[4-(1-pyrrolidinylmethyl)phenyl]-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 328546-49-2 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-5-methyl-2-[4-k]

(1H-pyrrol-1-ylmethyl)phenyl]-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 328546-50-5 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-(4-chlorophenyl)-5,6-dihydro-5-methyl-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 328546-51-6 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-(4-chlorophenyl)-5,6-dihydro-5-methyl-, (5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 328546-52-7 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-(4-chlorophenyl)-5,6-dihydro-5-(hydroxymethyl)-, (5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 328546-53-8 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4[(dimethylamino)methyl]phenyl]-5,6-dihydro-5-(hydroxymethyl)-, (5R)- (9CI)
(CA INDEX NAME)

RN 328546-54-9 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-5-(hydroxymethyl)-2-[4-[[methyl(2-phenylethyl)amino]methyl]phenyl]-, (5R)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 328546-55-0 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-5-(hydroxymethyl)-2-[4-[(methylamino)methyl]phenyl]-, (5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 328546-56-1 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-5-(hydroxymethyl)-2-[4-(1-pyrrolidinylmethyl)phenyl]-, (5R)- (9CI) (CF INDEX NAME)

RN 328546-57-2 CAPLUS

CN Benzeneacetonitrile, 4-(4,5,6,7-tetrahydro-7-oxoimidazo[4,5,1-jk][1,4]benzodiazepin-2-yl)- (9CI) (CA INDEX NAME)

RN 328546-58-3 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-[(2,5-dihydro-2,5-dimethyl-1H-pyrrol-1-yl)methyl]phenyl]-5,6-dihydro- (9CI) (CA INDEX NAME)

RN 328546-59-4 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-[(2,5-dimethyl-1H-pyrrol-1-yl)methyl]phenyl]-5,6-dihydro- (9CI) (CA INDEX NAME)

RN 328546-60-7 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-[1-(dimethylamino)ethyl]phenyl]-5,6-dihydro-(9CI) (CA INDEX NAME)

RN 328546-61-8 CAPLUS

Imidazo[4,5,1-jk][1,4] benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-[1-(1-k+1)]] and a simple of the context ofCN pyrrolidinyl)ethyl]phenyl]- (9CI) (CA INDEX NAME)

RN

328546-62-9 CAPLUS Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-[2-phenyl-1-(1-pyrrolidinyl)ethyl]phenyl]- (9CI) (CA INDEX NAME) CN

ΙT

328546-76-5P 328546-77-6P 328547-34-8P RL: BYP (Byproduct); PREP (Preparation)

(prepn. of tricyclic inhibitors of poly(ADP-ribose) polymerases)

328546-76-5 CAPLUS RN

Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[3-CN (dimethoxymethyl)phenyl]-5,6-dihydro- (9CI) (CA INDEX NAME)

328546-77-6 CAPLUS RN

CN (hydroxymethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 328547-34-8 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-[(1E)-2-phenylethenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 328546-96-9 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-[2-[(methylsulfonyl)oxy]ethoxy]phenyl]- (9CI) (CA INDEX NAME)

RN 328547-10-0 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-(chloromethyl)phenyl]-5,6-dihydro- (9CI) (CA INDEX NAME)

RN 328547-13-3 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-(chloromethyl)phenyl]9-fluoro-5,6-dihydro- (9CI) (CA INDEX NAME)

RN 328547-15-5 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-(hydroxymethyl)phenyl]-5-methyl-, (5S)- (9CI) (CA INDEX NAME)

RN 328547-16-6 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-(chloromethyl)phenyl]-5,6-dihydro-5-methyl-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 328547-17-7 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-(2-chloro-3-methylbutyl)phenyl]-5,6-dihydro- (9CI) (CA INDEX NAME)

RN 328547-21-3 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-(4-chlorophenyl)-5,6-dihydro-5-[(phenylmethoxy)methyl]-, (5R)- (9CI) (CA INDEX NAME)

RN 328547-23-5 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-(hydroxymethyl)phenyl]-5-[(phenylmethoxy)methyl]-, (5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 328547-24-6 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-(chloromethyl)phenyl]-5,6-dihydro-5-[(phenylmethoxy)methyl]-, (5R)- (9CI) (CA INDEX NAME)

RN 328547-25-7 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-(chloromethyl)phenyl]-5,6-dihydro-5-(hydroxymethyl)-, (5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 328547-26-8 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-(1-hydroxyethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 328547-28-0 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-(1-chloroethyl)phenyl]-5,6-dihydro-(9CI) (CA INDEX NAME)

RN 328547-30-4 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-(1-hydroxy-2-phenylethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 328547-32-6 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-(1-chloro-2-phenylethyl)phenyl]-5,6-dihydro- (9CI) (CA INDEX NAME)

IT 328546-89-0P 328547-22-4P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of tricyclic inhibitors of poly(ADP-ribose) polymerases)
328546-89-0 CAPLUS

RN 328546-89-0 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-(hydroxymethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 328547-22-4 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5-(bromomethyl)-2-(4-chlorophenyl)-5,6-dihydro-, (5R)- (9CI) (CA INDEX NAME)

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L16 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2002 ACS AN 1995:380741 CAPLUS DN 122:290829 TI Synthesis and Anti-HIV-1 Activity of 4,5,6,7-Tetrahydro-5methylimidazo[4,5,1-jk][1,4]benzodiazepin-2(1H)-one (TIBO) Derivatives. 3 Breslin, Henry J.; Kukla, Michael J.; Ludovici, Donald W.; Mohrbacher, ΑU Richard; Ho, Winston; Miranda, Milton; Rodgers, James D.; Hitchens, T. Kevin; Leo, Gregory; et al. CS Janssen Research Foundation, Spring House, PA, 19477, USA J. Med. Chem. (1995), 38(5), 771-93 SO CODEN: JMCMAR; ISSN: 0022-2623 DT Journal LΑ English GΙ

AΒ 4,5,6,7-Tetrahydro-5-methylimidazo[4,5,1-jk][1,4]benzodiazepin-2(1H)-ones (TIBO) (I, R = H, 5-Et, 7-Ph, etc.; X = S, 0; Y = 8-C1, 9-C1; Z = H, 3,3-dimethylallyl, Pr, etc.) have been shown to significantly inhibit HIV-1 replication in vitro by interfering with the virus's reverse transcriptase enzyme. We describe our synthetic endeavors around 4, 5, and 7 mono- and disubstitutions of I and discuss HIV-1 inhibitory structure-activity relationships. On the basis of inhibition of HIV-1 replication in MT-4 cells, we found that 5-mono-Me-substituted analogs and 7-mono-Me-substituted analogs of I were comparable as being consistently the most active compds. Although generally less active, the 4,5,7-unsubstituted, 4-mono-substituted, cis- and trans-5,7-di-Mesubstituted, and cis-4,5-di-Me-substituted analogs of I also exhibited significant activity. The remaining trans-4,5-di-Me-substituted, cis- and trans-4,7-di-Me-substituted, and all 4,5-, 5,6-, 6,7-, and 7,8-fused disubstituted analogs of I possessed no noticeable desired activity.

IT 162930-41-8P

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation) (synthesis and anti-HIV-1 activity of imidazobenzodiazepinones)

RN 162930-41-8 CAPLUS

CN Benz[b]imidazo[4,5,1-jk][1,4]benzodiazepin-6(7H)-one, 1,2-dihydro-1-thioxo-(9CI) (CA INDEX NAME)

10/041,556

TX 6

ANSWER 4 OF 5 CAPLUS COPYRIGHT 2002 ACS

1978:507034 CAPLUS

DN 89:107034

TI Fragmentation in mass spectrometry of imidazobenzodiazepines

AU Geneste, Patrick; Kamenka, Jean Marc; Vidal, Yves

CS Lab. Chim. Org. Phys. Appl., Ec. Natl. Super. Chim., Montpellier, Fr.

SO Org. Mass Spectrom. (1978), 13(3), 141-53 CODEN: ORMSBG; ISSN: 0030-493X

DT Journal

LA French

AB Mass spectra are reported for 7 imidazo[1,5,4-ef]-1,5- and 11 imidazo[4,5,1-jk]-1,4-benzodiazepines. Differences in fragmentation patterns enabled isomeric structures to be identified.

IT 66596-59-6 66596-60-9 RL: PRP (Properties)

(mass spectrum of)

RN 66596-59-6 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 9-chloro-5,6-dihydro-2-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 66596-60-9 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-9-nitro-2-(phenylmethyl)- (9CI) (CA INDEX NAME)

10/041,556

TX6

ANSWER 5 OF 5 CAPLUS COPYRIGHT 2002 ACS

1978:182987 CAPLUS

DN 88:182987

TI Studies on the imidazo[4,5,1-jk][1,4]benzodiazepine and imidazo[1,5,4-ef][1,5]benzodiazepine series

AU Geneste, P.; Kamenka, J. M.; Vidal, Y.; Fauquet, J. P.; Morel, E.; Muller, P.; Warolin, C.

CS Lab. Chim. Org. Phys. Appl., Ec. Natl. Super. Chim., Montpellier, Fr.

SO Eur. J. Med. Chem. - Chim. Ther. (1978), 13(1), 53-9 CODEN: EJMCA5

DT Journal ·

LA French

GI

AB Of the 7 title compds. (I and II, R = Me or PhCH2; X = O; Y = H, Cl, or NO2) prepd., none showed tranquilizing activity in pentetrazole-induced convulsions or mouse motor activity. The prepn. of I and II from imidazoquinolinones (III) is also described.

IT 66596-59-6P 66596-60-9P

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. and tranquilizing activity of)

III

RN 66596-59-6 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 9-chloro-5,6-dihydro-2-(phenylmethyl)- (9CI) (CA INDEX NAME)

Ph-CH₂
N
C1

RN 66596-60-9 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-9-nitro-2-

(phenylmethyl) - (9CI) (CA INDEX NAME)